HYDROGEN ATOM IN INTENSE MAGNETIC FIELD

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Abstract. The structure of a hydrogen atom situated in an intense magnetic field is investigated. Three approaches are employed. An elementary Bohr picture establishes a crucial magnetic field strength, $H_a \simeq 5 \times 10^9$ G. Fields in excess of H_a are intense in that they are able to modify the characteristic atomic scales of length and binding energy. A second approach solves the Schrödinger equation by a combination of variational methods and perturbation theory. It yields analytic expressions for the wave functions and energy eigenvalues. A third approach determines the energy eigenvalues by reducing the Schrödinger equation to a one-dimensional wave equation, which is then solved numerically. Energy eigenvalues are tabulated for field strengths of 2×10^{10} G and 2×10^{12} G. It is found that at 2×10^{12} G the lowest energy eigenvalue is changed from -13.6 eV to about -180 eV in agreement with previous variational computations.

1. Introduction

It is generally agreed that neutron stars are the seats of intense magnetic fields[1] ($\sim 10^{12}$ G). Many aspects of atomic structure are profoundly altered by such enormous fields – binding energies[2], opacities[3], etc. We suggest a thorough re-examination of 'conventional' atomic physics, imbedded in an intense magnetic field (IMF). As a step in this direction, we have made a detailed study of the hydrogen atom – a likely guide if the history of atomic theory is to repeat at 10^{12} G.

In keeping with historical precedent, we first present the Bohr theory. While subject to limitation, the Bohr picture may often be relied upon as a rule-of-thumb guide.

Our major effort combines analytic and numberical solutions of the Schrödinger equation. The analytic scheme is detailed in Sections 3–5. Approximate analytic wave functions and the corresponding energy spectra are established. In Section 6 we present the results of a combined analytical-numerical approach. There, the Schrödinger equation is reduced to a one-dimensional wave equation which is solved numerically. A comparison of the wave functions and energy spectra obtained by these two methods suggests that the analytic wave functions are sufficiently accurate for the calculation of many atomic properties.

2. Bohr Theory

The classic Bohr model is amended by imposing a uniform magnetic field, H. We assume that the electron and ion lie in the same plane and that they are tied to the same line of force. For an ion of infinite mass, the electron moves in a circular orbit of radius ϱ under the combined Coulomb and Lorentz forces. Equations (1)–(3) express New-

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ton's second law, the total electron energy, and the quantization of angular momentum,

$$\frac{mv^2}{\varrho} = \frac{eHv}{c} + \frac{e^2}{\varrho^2} \tag{1}$$

$$E = \tfrac{1}{2}mv^2 - \frac{e^2}{\varrho} \tag{2}$$

$$mv\varrho - \tfrac{1}{2}\frac{eH\varrho^2}{c} = (l+1)\,\hbar\,; \quad l = 1, 0, 2, \ldots. \tag{3}$$

The choice of $l+1$ as the angular momentum quantum number facilitates a subsequent comparison with the results of the Schrödinger equation analysis. It is convenient to introduce the Bohr radius, a_0, and energy, E_H, together with the cyclotron frequency, ω, and radius, R, defined as follows

$$
\begin{aligned}
a_0 &= \hbar^2/me^2\,; & E_H &= e^2/2a_0 = 13.6 \text{ eV} \\
\omega &= |e|\,H/mc\,; & R &= \sqrt{2\hbar/m\omega}
\end{aligned}
\tag{4}
$$

The discrete radii and energies which emerge as solutions of Equations (1)–(3) are determined by

$$(\varrho_l/a_0) + (\varrho_l/R)^4 = (l+1)^2 \tag{5}$$

$$E_l = \tfrac{1}{2}(l+1)\,\hbar\omega + \tfrac{1}{4}m\omega^2\varrho_l^2 - \frac{e^2}{2\varrho_l} \tag{6}$$

The binding energy of the electron is $-\varepsilon_b = E_H a_0/\varrho_0$. In the zero field limit, these expressions reduce to the historic results, $\varrho_l \to (l+1)^2 a_0$, $E_l \to -E_H/(l+1)^2$. An intense magnetic field may render $\varrho_l \ll a_0$, in which event the binding energy is increased greatly over the Bohr value. The field strength at which magnetic binding begins to dominate the Coulomb force is established by equating R and a_0. This transition to the IMF regime occurs at

$$H_a = 2m^2c\,(e/\hbar)^3 = 4.7 \times 10^9 \text{ G}. \tag{7}$$

For fields in excess of H_a, the orbits scale according to

$$\varrho_l \sim \sqrt{l+1}\,R\,, \tag{8}$$

and the binding energy becomes

$$-\varepsilon_b \approx E_H a_0/R\,. \tag{9}$$

If the field strength is expressed in units of 10^{12} G, the binding energy predicted by the Bohr model is

$$-\varepsilon_b \sim 280\,\sqrt{B_{12}}\text{ eV}. \tag{10}$$

The quantum treatment of Sections 3–4 suggests an orbit scale of $\varrho_l \approx \sqrt{(l+\tfrac{1}{2})}\,R$. The binding energy proves to be about twice the value obtained by numerical and variational solutions of the Schrödinger equation. The Bohr treatment is defective in that

it ignores motion parallel to the magnetic fields. The kinetic energy of the electron parallel to the field reduces the binding energy.

In summary, the Bohr picture establishes the crucial field strength ($H_a \sim 5 \times 10^9$ G), reveals the intense field orbit scale ($\varrho_l \sim \sqrt{(l+1)}\, R$), and hints at the binding energy.

3. Schrödinger Theory

The Schrödinger equations for an electron under the simultaneous presence of a constant uniform magnetic field and a Coulomb field is

$$\left\{ -\frac{\hbar^2}{2m}\left(\nabla - \frac{ie}{\hbar c}\mathbf{A} \right)^2 - \boldsymbol{\mu}\cdot\mathbf{B} - \frac{Ze^2}{r} \right\} \Psi(r) = E\Psi(r) \tag{11}$$

where

$$\mathbf{H} = \nabla \times \mathbf{A} \qquad \boldsymbol{\mu} = \frac{|e|\,\hbar}{2mc}\boldsymbol{\sigma} \tag{12}$$

H being the external magnetic field such that $H_x = H_y = 0$, $H_z = H$. When $Z = 0$, Equation (11) admits the well-known solution[4]

$$\Psi(r) = \frac{1}{\sqrt{L_3}}\, e^{ipz} \Phi_{ns}(xy) \tag{13}$$

where

$$\Phi_{ns}(xy) = \frac{e^{il\varphi}}{\sqrt{2\pi}}\sqrt{2\gamma}\, I_{ns}(\gamma\varrho^2); \quad n - s = l\,;$$

$$\varrho^2 = x^2 + y^2\,; \qquad \gamma = \tfrac{1}{2}\frac{H}{H_q}\frac{1}{\lambda_c^2} = \frac{1}{R^2}\,;$$

$$\lambda = \hbar/mc\,; \qquad H_q = m^2 c^3 / e\hbar\,; \quad I_{ns}(\xi^2) = \xi^{n-s} e^{-1/2\xi^2} Q_s^{n-s}(\xi^2) \times$$

$$\times (n!\, s!)^{-1/2}$$

$$\xi^2 = \gamma\varrho^2 = \varrho^2/R^2\,, \tag{14}$$

Q_α^β is the associated Laguerre polynomical; n is the principal quantum number and l the angular momentum number. The quantum number s has the geometrical interpretation of the distance of the center of the orbits from the origin. In Equation (13) the (x, y) and z coordinates separate because the magnetic field does not alter the z-motion of the particle.

It is evident from the $\exp(-\tfrac{1}{2}\varrho^2/R^2)$ structure of I_{ns} that the cyclotron radius R defines the radial scale of the probability distribution. In the IMF regime, R is much smaller than the Bohr radius. The result is a magnetic constriction of the familiar spherical electron distribution. The electron probability cloud become cigar-shaped. The Bohr radius fixes the scale of the charge distribution parallel to the field. The cyclotron radius plays the role of scale factor perpendicular to the field.

The magnetic constriction of the radial electron distribution is common to all states. This constriction produces a greatly enhanced binding only for the states in

which the wave function is without nodes in the z direction, i.e., parallel to the field. We refer to these nodeless states as tightly-bound because at field strengths in the 10^{12} G range, binding energies are well over 100 eV. The remaining states fall into two classes according to whether the z dependence of the wave function exhibits even or odd parity. We refer to these states as hydrogen-like because their energy spectra are quite similar to the familiar hydrogen spectrum.

The energy eigenvalues associated to the wave function (13) are[4]

$$\varepsilon = \hbar\omega\left(n + \sigma + \tfrac{1}{2}\right) + p_z^2/2m \qquad \begin{aligned} n &= 0, 1, 2, \ldots \\ \sigma &= \pm \tfrac{1}{2} \end{aligned} \tag{15}$$

$$= \varepsilon_\perp + p_z^2/2m \,.$$

In the absence of the Coulomb interaction, there is an infinite degeneracy: states with a given n and σ, but different s and l, have the same energy. This magnetic degeneracy of the electron energy is well-known. Our considerations are restricted to states with $n=0$, $\sigma=-\tfrac{1}{2}$, for which $\varepsilon_\perp=0$. In the IMF regime, all states have magnetic energies $\varepsilon_\perp$ far in excess of the Coulomb binding. Hence, bound states result only for $n=0$, $\sigma=-\tfrac{1}{2}$.

The Coulomb interaction removes the degeneracy, giving birth to an infinite set of tightly-bound states and to a doubly infinite set of hydrogen-like states. The tightly-bound states correspond to those discovered in the Bohr theory. For these states, the z-dependent portion of the wave function is without nodes and has a maximum at $z=0$. In Section 4 we develop a variational solution for these tightly-bound states. In addition to the tightly-bound states there are states for which the z-dependent portion of the wave function resembles closely the solutions of the one-dimensional Schrödinger equation with a potential $-e^2/(|z|+b)$. That is, it resembles the solutions of a one-dimensional wave equation for a truncated Coulomb potential [5, 6]. In Section 5 these solutions are used as the basis for a perturbation solution.

4. Tightly-Bound States

For states with $n=0$, $(s=-l=0; 1, 2, \ldots)$, a variational computation is performed with a trial function of the form* (for $n=0$, the Laguerre polynomials reduce to a constant).

$$\Psi = B_s \xi^s e^{-1/2\xi^2} e^{-is\varphi} f(z) \,. \tag{16}$$

For $f(z)$ we adopt[7]

$$f(z) = A_s e^{-1/2\lambda^2 z^2/R^2} \tag{17}$$

where λ is the variational parameter. The tightly-bound states have $\varepsilon_\perp=0$ and their energy is therefore given by

$$E_s = \frac{h^2}{2m} \int \left(\frac{\partial f}{\partial z}\right)^2 \mathrm{d}z - e^2 \int \frac{|\Psi|^2 \, \mathrm{d}^3 r}{\sqrt{\varrho^2 + z^2}} \,. \tag{18}$$

* The radial probability distribution varies as $\xi^{2s+1}e^{-\xi}$. This has a maximum at $\xi=\sqrt{s+\tfrac{1}{2}}$ or $\varrho= R\sqrt{s+\tfrac{1}{2}}$ which may be compared with the $R\sqrt{(s+1)}$ scale of the IMF limit of Bohr theory.

The variational method is applicable to all of the tightly-bound states – not just the ground state – provided the trial function for the sth excited state is orthogonal to all of the exact eigenstate of lower energy. This is guaranteed here by the $e^{-is\varphi}$ factor which appears in the exact eigenfunctions as well as in our trial functions.

Performing the necessary integration the energies are given (in units of $E_H = 13.6\,\mathrm{eV}$)

$$E_s = \left[\tfrac{1}{2}\lambda_s^2 - \frac{2R\lambda_s}{a_0\sqrt{\pi}} I_s(\lambda_s) \right] \left(\frac{a_0}{R} \right)^2 , \tag{19}$$

with λ_s fixed by the condition $\partial E_s / \partial \lambda = 0$. $I_s(\lambda)$ is given by

$$I_s(\lambda) = \int_0^\pi \frac{(\sin\theta)^{2s+1}\,\mathrm{d}\theta}{(\sin^2\theta + \lambda^2 \cos^2\theta)^{s+1}} . \tag{20}$$

The evaluation of the I_s is not difficult, but their unwieldy form complicates the task of fixing the E_s. Fortunately, the λ_s are small in the IMF regime, permitting the approximations,

$$\left. \begin{aligned} I_0 &\approx 2\log(2/\lambda) \\ I_s &\approx I_0 - \sum_{k=1}^s \frac{1}{k} \quad s \geqslant 1 \end{aligned} \right\} \lambda^2 \ll 1 \tag{21}$$

Imposing the variational constraint leads to

$$E_s = -\lambda_s \left[\frac{4R}{a_0\sqrt{\pi}} + \tfrac{1}{2}\lambda_s \right] \left(\frac{a_0}{R} \right)^2 , \tag{22}$$

where λ_s is the solution of the following transcendental equation

$$\lambda_s = \frac{4R}{a_0\sqrt{\pi}} \left[\log\left(\frac{2}{\lambda_s} \right) - 1 - \tfrac{1}{2}A_s \right] ,$$

$$A_0 = 0 ; \quad A_s = \sum_{k=1}^s \frac{1}{k} \quad s \geqslant 1 . \tag{23}$$

For a field strength of 2×10^{12} G, Equation (22) gives $-E_0 = 13.5\,(\approx 183\,\mathrm{eV})$ for the ground state binding energy, about 4% shy of the value 14.0 obtained in Section 6 from a numerical solution of the wave equation. The spectrum of tightly-bound states forms an infinite sequence which approaches the continuum $(s \to \infty)$ as $s^{-1/2}$.

5. Hydrogen-Like States

To deal with the hydrogen-like states we adopt a perturbation theory approach. The actual potential $-e^2/r$ is replaced by the one-dimensional potential $-e^2/(|z|+d)$ and their difference is treated as a perturbation. For the zero-order wave functions we take

$$\Psi = C_\sigma f(z) I_{ns}(\xi^2) e^{-is\varphi} \tag{24}$$

where $f(z)$ is a solution of

$$-\frac{h^2}{2m}\frac{d^2 f}{dz^2} - \frac{e^2}{|z| + d} f = E_z f.$$ (25)

The length parameter, d, is at our disposal. The total energy, through first order in the perturbation is

$$E = E_z + \langle V \rangle,$$ (26)

where

$$\langle V \rangle = -e^2 \int \frac{|\Psi|^2 \, d\tau}{r} + e^2 \int \frac{f^2 \, dz}{|z| + d}.$$ (27)

Again, we have assumed that Ψ and $f(z)$ are separately normalized to unity.

The solutions of (25) may be expressed in terms of Whittaker function, $W_\beta(\zeta)$ [5, 6, 8].

$$f(z) = B W_\beta(\zeta); \quad \zeta \equiv \frac{2z}{\beta a_0} + \frac{2d}{\beta a_0}.$$ (28)

The power series form of the Whittaker functions is

$$W_\beta(\zeta) = \frac{e^{-1/2\zeta}}{\Gamma(-\beta)} \left(-\frac{1}{\beta} + \sum_{r=1}^{\infty} \lambda_r \zeta^{r+1} + [\log \zeta + K_\beta] \sum_{l=0}^{\infty} \alpha_r \zeta^{r+1} \right)$$ (29)

with the various coefficients given by

$$\alpha_r = \frac{(1-\beta)_r}{r!\,(r+1)!}; \quad (1-\beta)_r = (1-\beta)(2-\beta)\ldots(r-\beta)$$

$$\lambda_r = \alpha_r \sum_{n=0}^{r-1} [(n+1-\beta)^{-1} - (n+1)^{-1} - (n+2)^{-1}]$$

$$K_\beta = \Psi(1-\beta) - \Psi(1) - \Psi(2),$$

$\Psi(x)$ is the logarithmic derivative of the gamma function. The index β (and through it the energy spectrum) is determined by the boundary condition imposed on $f(z)$ at the origin. Taking $f(0)=0$ results in states of odd parity; requiring $df/dz|_{z=0}=0$ generates the states of even parity. The energy E_z is related to β by

$$E_z = -E_H/\beta^2.$$ (30)

The values open to β depend on the parameter d. We propose that a judicious choice for d is one which renders $\langle V \rangle = 0$. The energy then differs from the unperturbed value only in second order. Unfortunately, it is not possible to obtain an analytic expression for $\langle V \rangle$ (and thus our desire to avoid it entirely!). This forces us to resort to guess-work of a sort. The actual scheme for assigning d a value will be discussed shortly. For the moment it suffices to note that we can safely assume $d/a_0 \ll 1$. This follows because d *somehow* measures the radial probability distribution whose scale is $R \ll a_0$. With $d/a_0 \ll 1$, the eigenvalue equations lead to values of β close to the positive integers.

Following a scheme detailed by Loudon[5], we find, for states of odd parity,

$$\beta_{\text{odd}} = p + 2d/a_0 ; \qquad p = 1, 2, 3, \ldots, \tag{31}$$

while for states of even parity,

$$\beta_{\text{even}} = p + \frac{1}{t + \sqrt{t^2 + \pi^2/3}} ; \qquad p = 1, 2, 3, \ldots, \tag{32}$$

with

$$t = -0.58 - d/a_0 - \tfrac{1}{2} \log(2d/a_0) + \frac{1}{24p^2} . \tag{33}$$

As noted above, the value assigned to the parameter d is to be such that $\langle V \rangle = 0$. We now give consideration as to how this may be accomplished. The number of nodes in the z direction* equals the index p. The turning point of $W_{\beta \approx p}$ occurs at $z = 2p^2 a_0$. There is a roughly uniform spacing of nodes and antinodes, with none beyond the turning point. Thus, the node-antinode spacing is approximately pa_0. For states of even parity, the first node should lie near $z = pa_0$. The condition that $\langle V \rangle = 0$ is

$$\int_0^\infty \frac{f^2 \, dz}{z + d} = \int_0^\infty \frac{\theta^s e^{-\theta} \, d\theta}{s!} \int_0^\infty \frac{f^2 \, dz}{\sqrt{z^2 + R^2 \theta}} \tag{34}$$

For $z \gtrsim pa_0$, the z integrands are virtually equal. The integral on the left receives a substantial contribution from the range $0 \leqslant z \leqslant z_0$, where z_0 is several times d, but $z_0 \ll pa_0$. Over this narrow range, we may take $f^2 \approx \text{const}$.

With these approximations, (34) reduces to

$$\log\left(\frac{z_0}{d}\right) \approx \int_0^\infty \frac{\theta^s e^{-\theta} \, d\theta}{s!} \log\left(\frac{2z_0}{R\sqrt{\theta}}\right) .$$

The parameter z_0 drops out leaving

$$2 \log\left(\frac{R}{2d}\right) = \begin{cases} \log \gamma - \displaystyle\sum_{k=1}^s \frac{1}{k} & s \geqslant 1 \\[2mm] \log \gamma ; \quad s = 0 ; \quad \gamma = 0.577 \ldots . \end{cases}$$

For our purposes, the sum $\displaystyle\sum_{k=1}^s 1/k$ is adequately approximated by $\log(s+1)$; whence, for states of even parity, we find that d is directly proportional to R

$$d_{\text{even}} = \sqrt{\frac{s+1}{\gamma}} \frac{R}{2} . \tag{35}$$

For odd parity states, over the range $0 \leqslant z \leqslant pa_0$, where the z integrands differ, $f(z)$ is

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* Between 0 and infinity. For odd parity states this counts the node at the origin.

roughly proportional to z. If, in addition, we replace ϱ^2 by its mean value $(s+1)R^2$, the condition $\langle V \rangle = 0$ requires

$$\int_0^{pa_0} \frac{z^2\,dz}{z+d} = \int_0^{pa_0} \frac{z^2\,dz}{\sqrt{z^2 + (s+1)R^2}}.$$

This yields

$$d_{\text{odd}} = \frac{pa_0}{\lambda}\left[\log\lambda - 1\right]; \quad \lambda = \frac{4p^2 a_0^2}{(s+1)R^2}. \tag{36}$$

The even and odd parity energy spectra are given by (in units of E_H)

$$E_{p,s}^{(\text{even})} = -\left(p + \frac{1}{t + \sqrt{t^2 + \pi^2/3}}\right)^{-2},$$

$$E_{p,s}^{(\text{odd})} = -\left(p + \frac{2p}{\lambda}\left[\log\lambda - 1\right]\right)^{-2}. \tag{37}$$

The parameters t and λ are defined by Equations (33) and (36), respectively. For a field strength of 2×10^{12} G,

$$t = 0.80 - \tfrac{1}{4}\log(s+1) + \frac{1}{24p^2}$$

$$\lambda = 1696\,p^2/(s+1).$$

6. Exact Numerical Solutions

As we said before, the Schrödinger equation for an electron under the simultaneous presence of a constant uniform magnetic field and a Coulomb field, does not admit exact analytic solutions since the cylindrical and spherical symmetry of the problem does not allow a separation of variables. These technical problems prompted Schiff and Snyder [9] as early as 1939 to introduce the so-called adiabatic approximation described below. In Equation (13) the (x, y) and z coordinates separate because the magnetic field does not alter the z-motion of the particle. The adiabatic hypothesis consists of taking the exact wave function $\Psi(r)$ as a linear superposition of function of the form (13) with $\exp(ipz)$ changed into a new function $f(z)$ to be determined. Physically, the assumption that the variables do separate even in the presence of a Coulomb field, is equivalent to saying that the strongly quantized orbits in the x-y plane are not changed by the Coulomb field. That this is a good line of approach is fully justified by the preceding arguments. Let us therefore write

$$\Psi(r) = \sum_\alpha c_\alpha f_\alpha(z)\,\Phi_\alpha(xy) \tag{38}$$

where α is the set of quantum numbers n and l. Substituting it back into Equation (11) we obtain

$$\sum_\alpha c_\alpha \Phi_\alpha(xy)\left[\varepsilon_\perp^\alpha - \frac{\hbar^2}{2m}\nabla_z^2 - \frac{e^2}{r}\right]f_\alpha(z) = E\sum_\alpha c_\alpha \Phi_\alpha(xy)\,f_\alpha(z), \tag{39}$$

where $\varepsilon_\perp^\alpha$ is given by Equation (15).

Multiplying Equation (39) by Φ_β^* from the left and integrating on x and y, the result is

$$c_\beta \varepsilon_\perp^\beta f_\beta(z) - \frac{\hbar^2}{2m} \nabla_z^2 f_\beta(z) - e^2 \sum_\alpha c_\alpha \int dx\, dy\, \frac{\Phi_\beta^*(xy)\, \Phi_\alpha(xy)}{r} f_\alpha(z) =$$
$$= E c_\beta f_\beta(z); \quad (40)$$

or $(\nabla_z^2 \equiv \nabla^2)$ defining a one-dimensional potential $V_{\alpha\beta}$ as

$$V_{\alpha\beta}(z) = e^2 \int dx\, dy\, \frac{\Phi_\alpha^*(xy)\, \Phi_\beta(xy)}{r} \quad (41)$$

with

$$\left[+\frac{\hbar^2}{2m} \nabla^2 + \sum_\alpha \frac{c_\alpha}{c_\beta} V_{\alpha\beta}(z) \right] f_\beta(z) = \tilde{E}_\beta f_\beta(z), \quad (42)$$

$$\tilde{E} = -E + \varepsilon_\perp^\beta. \quad (43)$$

Equation (42) is a one-dimensional Schrödinger equation or more properly an infinite set of coupled Schrödinger equations. Such a problem is well-known in quantum chemistry and refined methods have purposely been developed to handle the situation. The number of coupled equations to be solved strongly depend on the degree of over-lapping of the Φ's. Looking back to Equation (14) we see that the higher H, the higher the degree of overlapping since these wave functions contain a Gaussian $e^{-\gamma \varrho^2}$. The degree of overlapping could be slightly perturbed by the presence of the Laguerre polynomial. On the other hand, it is clear from Equation (43) that the only sizeable effect should occur at $n=0$, $\sigma=-\frac{1}{2}$, i.e., at zero transverse energy, since otherwise the 'atomic part' or the spectrum (z-direction) which we expect to be of the order/of some tens of eV will be negligible with respect to the $\perp$ energy that for $H/H_q \simeq 1$ is of the order of 1 MeV. For these reasons we will approximate

$$\sum_\alpha c_\alpha V_{\alpha\beta} \approx c_\beta V_{\beta\beta}$$

and Equation (42) takes the form

$$\left[+\frac{\hbar^2}{2m} \nabla^2 + V_{ns}(z) \right] f_p(z) = \tilde{E}_p f_p(z). \quad (44)$$

Given a set of quantum numbers, n and s, we will compute $V_{ns}(z)$ and consequently the eigenvalue $\tilde{E}$: since they are quantized we will characterize them by the index p.

7. The One-Dimensional Coulomb Potential

From the definition of $V_{ns}(z)$, Equation (41) and the form of the wave functions $\Phi(x, y)$, Equation (14), we have ($x=r \cos \varphi$, $y=r \sin \varphi$)

$$V_{ns}(z) = e^2 \gamma \int_0^\infty r\, dr\, \frac{1}{\sqrt{z^2 + r^2}} I_{ns}^2(\gamma r^2) = e^2 \sqrt{\gamma} \int_0^\infty dx\, \frac{I_{ns}^2(x)}{\sqrt{x^2 + \gamma z^2}}. \quad (45)$$

Since $(x + \alpha^2)^{-1/2}$ is the Laplace transorm of the Bessel function of the order zero, i.e.,

$$\frac{1}{\sqrt{x + \alpha^2}} = \int_0^\infty \mathrm{d}y\, e^{-\alpha y} J_0\left(y\sqrt{x}\right)$$

Equation (45) becomes

$$V_{ns}(z) = e^2 \sqrt{\gamma} \int_0^\infty e^{-yz\sqrt{\gamma}} I_{nn}\left(y^2/4\right) I_{ss}\left(y^2/4\right) \mathrm{d}y, \qquad (46)$$

where we have used the fundamental relation [4]

$$\int_0^\infty \mathrm{d}x\, I_{\alpha\beta}(x)\, I_{\gamma\delta}(x)\, J_{(\alpha-\beta)-(\gamma-\delta)}\left(2\sqrt{Ax}\right) = I_{\alpha\gamma}(A)\, I_{\beta\delta}(A).$$

Equation (46), although still very difficult to compute, is in a much better form since we have separated the indices n and s whose physical significance is entirely different. For practical purposes, Equation (46) can be cast in a varity of forms. First of all, it is convenient to rewrite Equation (44) in atomic units, i.e.,

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}z^2} + V_{ns}(z)\right] f_p(z) = E_p f_p(z), \qquad (47)$$

with

$$z = z/a_0, \quad E_p = -\tilde{E}_p/E_H,$$

$$V_{ns}(z) = \frac{z}{\alpha} \sqrt{\frac{H}{2H_q}} \int_0^\infty e^{-\lambda y} \mathrm{d}y\, I_{nn}\left(y^2/4\right) I_{ss}\left(y^2/4\right), \qquad (48)$$

$$\lambda = \frac{1}{\alpha} \sqrt{\frac{H}{2H_q}}\, z; \quad \alpha = e^2/\hbar c.$$

Using the definition of the $I_{\alpha\beta}$ functions of Equation (14), we obtain

$$V_{ns}(z) = \frac{4}{\alpha} \sqrt{\frac{H}{2H_q}} \sum_{p=0}^{n} \sum_{q=0}^{s} \frac{(-)^{p+q}}{4^{p+q}} \binom{n}{n-p}\binom{s}{s-q} \frac{1}{p!\,q!} \times$$

$$\times \frac{\mathrm{d}^{2(p+q)}}{\mathrm{d}\lambda^{2(p+q)}} \left[e^{\lambda^2} \mathrm{ERFC}\,\lambda\right], \qquad (49)$$

where

$$\mathrm{ERFC}\, x = \int_x^\infty e^{-y^2}\, \mathrm{d}y.$$

For $n = s = 0$, Equation (49) simply becomes

$$V_{00}(z) = \frac{4}{\alpha} \sqrt{\frac{H}{H_q}} \, e^{\lambda^2} \, \text{ERFC} \, \lambda \tag{50}$$

which is exactly Equation (12) of Schiff and Snyder [9].
Using a rational approximation to ERFC(8), we obtain

$$e^{x^2} \, \text{ERFC} \, x = (1 - \text{ERF} \, x) \, e^{x^2} =$$

$$= \frac{a_1}{1 + \varrho x} + \frac{a_2}{(1 + \varrho x)^2} + \frac{a_3}{(1 + \varrho x)^3} + \frac{a_4}{(1 + \varrho x)^4} + \frac{a_5}{(1 + \varrho x)^5} \tag{51}$$

with

$$\varrho = 0.327 \quad a_1 = 0.255 \quad a_2 = -0.284 \quad a_3 = 1.421$$
$$a_4 = -1.45 \quad a_5 = 1.06.$$

We see that the first term is exactly the truncated Coulomb potential used in Section 5, Equation (25). Inclusion of the second term in expansion (51) would still allow an exact solution of Equation (25) in terms of Whittaker function with two indices.

Equation (47) was solved numerically for $n=0$, $s=0, 1, 2, \ldots 5$ at $H=2 \times 10^{12}$ and $H=2 \times 10^{10}$ G. The results are shown in Tables I–VI.

TABLE I

The table entries are the binding energies in units of $E_H = -13.6$ eV. The numbers in parenthesis were obtained using Equation (22) or Equation (37). All others were obtained by the numerical method outlined in the Appendix. Tables I – III give results for a field strength of 2×10^{12} G. Tables IV – VI convey the results for 2×10^{10} G.

$n=s=0$ Even	Odd	$n=0, s=1$ Even	Odd
	0.0203		0.0202
0.0251		0.0248	
	0.0277		0.0270
0.0354		0.0349	
	0.040		0.0398
0.0538		0.0529	
	0.061		0.0621
0.091		0.0892	
(0.089)		(0.0870)	
	0.111		0.110
	(0.111)		(0.111)
0.187		0.181	
(0.180)		(0.175)	
	0.248		0.247
	(0.249)		(0.248)
0.58		0.552	
(0.548)		(0.520)	
	0.988		0.972
	(0.984)		(0.968)
14.0		10.6	
(13.5)		(10.0)	

TABLE II

$n=0, s=2$ Even	Odd	$n=0, s=3$ Even	Odd
	0.0202		0.0269
0.0246		0.0344	
	0.0276		0.0397
0.0346		0.0520	
	0.0397		0.0618
0.0524		0.0872 (0.085)	
	0.0610		0.109 (0.110)
0.0880 (0.086)		0.176 (0.170)	
	0.110 (0.111)		0.244 (0.246)
0.178 (0.172)		0.521 (0.496)	
	0.245 (0.247)		0.953 (0.944)
0.534 (0.508)		8.15	
	0.962 (0.956)		
9.09 (8.50			

TABLE III

$n=0, s=4$ Even	Odd	$n=0, s=5$ Even	Odd
	0.0269		0.0268
0.0342		0.0341	
	0.0396		0.040
0.0517		0.0514	
	0.0617		0.0616
0.0865 (0.084)		0.0860 (0.084)	
	0.109 (0.110)		0.109 (0.110)
0.173 (0.168)		0.172 (0.166)	
	0.243 (0.245)		0.242 (0.244)
0.512 (0.488)		0.503 (0.480)	
	0.945 (0.936)		0.937 (0.924)
7.50		7.01	

TABLE IV

$n=0, s=0$ Even	Odd	$n=0, s=1$ Even	Odd
0.0321		0.0309	
	0.0378		0.0369
0.0479		0.0459	
	0.0568		0.0565
0.0784		0.0742	
	0.101		0.0970
0.151		0.140	
	0.217		0.204
0.405		0.355	
	0.748		0.659
3.14		2.07	

TABLE V

$n=0, s=2$ Even	Odd	$n=0, s=3$ Even	Odd
0.0302		0.0297	
	0.0362		0.0357
0.0447		0.0439	
	0.0552		0.0543
0.0719		0.0702	
	0.0942		0.0921
0.134		0.130	
	0.195		0.189
0.330		0.313	
	0.605		0.567
1.69		1.46	

TABLE VI

$n=0, s=4$ Even	Odd	$n=0, s=5$ Even	Odd
0.0294		0.0290	
	0.0353		0.0349
0.0433		0.0428	
	0.0535		0.0529
0.0690		0.0679	
	0.0904		0.0890
0.126		0.124	
	0.183		0.179
0.300		0.290	
	0.538		0.515
1.32		1.21	

8. Conclusions

Various considerations are in order just by looking at the preceding tables.

(1) For a fixed value of s the energy of the tightly-bound state is greatly depressed in comparison with the hydrogen-like state energies. For fields in the 10^{12} G range the separation exceeds 100 eV.

(2) With increasing s, the binding energy of the tightly-bound states decrease. The decline exhibited by the tabulated values is somewhat more rapid than the $s^{-1/2}$ behavior deduced from the Bohr theory. For large s the variational calculation leads to the same $s^{-1/2}$ spectrum. At a field strength of 2×10^{12} G a simple calculation shows that a value of $s \approx 100$ is needed to give a binding energy comparable to the zero-field value of 13.6 eV.

(3) Overall, the effect of an IMF on the hydrogen-like states is to group them according to their parity with respect the field direction. Eigenvalues for states of odd parity follow closely the law $1/p^2$, $p = 1, 2, 3, \ldots$. The even parity states form a hydrogen-like sequence with a 'quantum defect', δ, which is only weakly dependent on the quantum numbers s and p. The even parity eigenvalues vary as $1/(p+\delta)^2$, $p = 1, 2, 3 \ldots$.

(4) In Tables I–III, we have also quoted, in parentheses, the values obtained using the analytic expressions given by Equation (37) or the variational results of Equation (22).

A comparison of the z-dependent portion of the wave functions reveals differences of less than 5% in values of the antinode amplitudes and positions of/the nodes and antinodes. Complete agreement is of course not to be expected since the two potentials are not identical.

Acknowledgements

Appendix

NUMERICAL METHOD

The solutions of the Schrödinger equation are computed over the range $(0 \leqslant z < \infty)$, instead of $(-\infty < z < \infty)$, the actual range, since they are odd or even over the latter range. The boundary conditions at $z=0$ are

$$f(z)\big|_{z=0} = 0 \quad \text{(odd)},$$
$$\frac{df}{dz}\Big|_{z=0} = 0 \quad \text{(even)}.$$

In practice however, the second condition is replaced by

$$f(z) \sim C \cos kz,$$
$$k = \sqrt{V(0) - E},$$

which follows from the fact that V behaves as a constant near $z = 0$. This is necessary for the particular method chosen to solve the differential equation. At $z = \infty$, the other boundary point, the solution becomes

$$f(z) = CW_{\alpha, 1/2}(\zeta) \sim \zeta^\alpha e^{-\zeta/2},$$
$$\alpha = A/2\sqrt{E}, \qquad \zeta = 2\sqrt{E}z,$$

where $W_{\alpha\beta}$ is Whittaker's confluent hypergeometric function since here the potential behaves like a Coulomb potential for large z, i.e.,

$$V(z) \underset{z \to \infty}{\sim} -\frac{A}{z}.$$

The integration of the differential equation follows the method of Numerov which applies to equations of the form $y'' = q(x)y$ of which the Schrödinger equation is such a type. y_{ij} (the value at x_j) is computed as an algebraic function of y_{j-1}' y_{j-2} and $q(x)$ at the respective points.

The energy E is obtained by making a guess close to what one believes is the true energy corresponding to a given number of nodes. A correction formula which gives a new energy in terms of the old and the discontinuities in the solution and its derivative at the classical turning point (where $V(z) - E = 0$) is applied repeatedly until the discontinuities disappear.[10]

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